

ON NEWTON-LIKE GUMMEL ITERATIVE SOLUTIONS TO DRIFT-DIFFUSION EQUATIONS

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Abstract

The one-dimensional carrier transport equations as they apply to the semiconductor devices are governed by the one-dimensional drift-diffusion model. It is defined by the Poisson's equation, the electron continuity equation and finally the hole continuity equation. The scaled Poisson's equation is (under standard notations)

$$\lambda^2 \frac{\partial^2 \psi(x,t)}{\partial x^2} - n(x,t) + p(x,t) + C(x) = 0$$

The concentrations of carriers in a semiconductor are given by

$$\frac{\partial J_n}{\partial x} - \frac{\partial n}{\partial t} - R = 0, \quad J_n = \mu_n \left(\frac{\partial n}{\partial x} - n \frac{d^2 \psi}{dx^2} \right)$$

and

$$\frac{\partial J_p}{\partial x} + \frac{\partial p}{\partial t} + R = 0, \quad J_p = -\mu_p \left(\frac{\partial p}{\partial x} - p \frac{d^2 \psi}{dx^2} \right)$$

where J_n and J_p are the current densities for the electrons and holes respectively.

When finite difference modelling for the partial differential equations is employed, nonlinear relations of the nodes accrue. This system of nonlinear equations is then solved by the Newton-Raphson method or by the Gummel iterative procedure. These results enable us to gain insights for the design of better numerical techniques.

Keywords: drift-diffusion equations, Gummel iteration, Newton-Raphson.

1. Introduction

The standard transport theory has been based on the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \frac{e\mathbf{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = \sum_{\mathbf{k}'} \{ S(\mathbf{k}', \mathbf{k}) f(\mathbf{r}, \mathbf{k}', t) [1 - f(\mathbf{r}, \mathbf{k}, t)] - S(\mathbf{k}, \mathbf{k}') f(\mathbf{r}, \mathbf{k}, t) [1 - f(\mathbf{r}, \mathbf{k}', t)] \} \quad (1)$$

where \mathbf{r} is the position, \mathbf{k} is the momentum, $f(\mathbf{r}, \mathbf{k}, t)$ is the distribution function, \mathbf{v} is the group velocity, \mathbf{E} is the electric field, $S(\mathbf{k}, \mathbf{k}')$ is the transition probability between the momentum states \mathbf{k} and \mathbf{k}' , and $[1 - f(\mathbf{r}, \mathbf{k}', t)]$ is the probability of non-occupation for a momentum state \mathbf{k}' .

Device simulations are normally based on the numerical solution of approximate models which are related to the Boltzmann equation, coupled to Poisson's equation for self-consistency.

In the simplest approach, the collision term on the right hand side of (1) is substituted with a *phenomenological* term

$$\frac{f_{eq} - f(\mathbf{r}, \mathbf{k}, t)}{\tau} \quad (2)$$

where f_{eq} indicates the (local) equilibrium distribution function, and τ is a microscopic relaxation time. For computational ease of electrical current calculation, velocity is used. In equilibrium and where degeneracy is absent, we may use the Maxwell-Boltzmann distribution function

$$f_{eq}(\mathbf{r}, \mathbf{v}) = n(\mathbf{r}) \left(\frac{2\pi k_B T_0}{m^*} \right)^{-3/2} \exp \left(- \frac{m^* |\mathbf{v}|^2}{2k_B T_0} \right) \quad (3)$$

where $n(\mathbf{r})$ is the carrier density, T_0 is the lattice temperature, k_B is the Boltzmann constant, and m^* is the effective mass. The carrier density, $n(\mathbf{r})$ is

$$n(\mathbf{r}) = \int d\mathbf{v} f(\mathbf{r}, \mathbf{v}) \quad (4)$$

If the electric field is switched off instantaneously and a space-independent distribution is considered, the resulting Boltzmann equation becomes

$$\frac{\partial f}{\partial t} = \frac{f_{eq} - f}{\tau} \quad (5)$$

Using $m^* \mathbf{v} = \hbar \mathbf{k}$, we have

$$\frac{e\mathbf{E}\partial f}{m^* \partial \mathbf{v}} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{f_{eq} - f}{\tau} \quad (6)$$

and using the general definition of current density which is given by

$$\mathbf{J}(\mathbf{x}) = e \int f(\mathbf{v}, \mathbf{x}) d\mathbf{v}$$

(7)

we obtain

$$-\frac{\mathbf{J}(\mathbf{x})}{e\tau} = \frac{1}{\tau} \int \mathbf{v} f_{eq} d\mathbf{v} - \int f(\mathbf{v}, \mathbf{x}) d\mathbf{v} \quad (8)$$

The equilibrium distribution function is symmetric in \mathbf{v} , and its integral is zero. Therefore, we have

$$\mathbf{J}(\mathbf{x}) = -e \frac{e\tau}{m^*} \mathbf{E} \int \mathbf{v} \frac{\partial f}{\partial \mathbf{v}} d\mathbf{v} - e\tau \frac{d}{dx} \int \mathbf{v}^2 f(\mathbf{v}, \mathbf{x}) d\mathbf{v} \quad (9)$$

Using elementary calculus and some simplifications, we are able to get the expressions for the drift-diffusion equations as given below. Details of the derivations of the drift diffusion equations can be found in Selberherr (1984).

2. Continuous Drift Diffusion Equations

In this section we shall obtain the basic semiconductor equations which describe the behaviour of a semiconductor device in terms of the electrostatic potential, the carrier concentrations and the current flow.

The fundamental physical equations for electromagnetic field calculations are the Maxwell equations:

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \quad (10)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (11)$$

$$\nabla \cdot \mathbf{D} = \rho \quad (12)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (13)$$

where

\mathbf{E} is the electric field strength vector, \mathbf{D} is the electric flux density vector, \mathbf{B} is the magnetic flux density vector, \mathbf{H} is the magnetic field strength vector, \mathbf{J} is the current density vector and ρ is the charge density.

Using equations (11), (12) and (13), we are able to get the Poisson's equation

$$\nabla^2 \psi = q(n - p + C) \quad (14)$$

with

$$\rho = q(p - n + C) \quad (15)$$

$C(x, t)$ is the doping function but usually it is a function of position only.

The continuity equations are the conservation laws for the carriers, namely the electrons and the holes. n and p are the concentrations of the electron and hole respectively, and μ_n and μ_p are their conductivities. The current equations describe the carrier drift due to external electric field \mathbf{E} and their diffusion due to the concentration gradient of the charges which are determined by their diffusion constants D_n and D_p respectively.

R_n and R_p are the net generation-recombination rates.

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + R_n \quad (16)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + R_p \quad (17)$$

$$\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n \quad (18)$$

$$\mathbf{J}_p = qp\mu_p \mathbf{E} + qD_p \nabla p \quad (19)$$

The problem (one-dimensional) is then completely defined with the assignment of boundary conditions.:

$$\begin{aligned} n(x, 0) &= n_D \\ p(x, 0) &= p_D \\ \psi(x, 0) &= \psi_D, \quad x \in \partial\Omega_D \\ \nabla \psi \cdot \mathbf{u} &= \mathbf{J}_n \cdot \mathbf{u} = \mathbf{J}_p \cdot \mathbf{u}, \quad \mathbf{u} \in \partial\Omega_N \end{aligned} \quad (20)$$

$\hat{\mathbf{u}}$ is the unit normal vector to the boundary. The boundaries consist of ohmic contacts, $\partial\Omega_D$ and physical or artificial surfaces $\partial\Omega_N$.

3. On Newton-like Gummel's Solution Procedures

Direct numerical methods for device simulation become more restrictive when the equations become more complex as its dimension increases. The complete 3-D time-dependent form requires seven independent variables for time, space and momentum. We may simulate using Monte Carlo technique which involves the simulation of particle trajectories or may solve the partial differential equations directly, Bank et. al (1981), (1982). Finite difference modelling imposes a uniform mesh and approximations are made at each interior node by a finite difference formula. The finite difference scheme gives relations of the nodes such as

i) Potential

$$\frac{2\lambda^2}{h_i(h_{i-1} + h_i)}(\psi_{i+1} - \psi_i) - \frac{2\lambda^2}{h_{i-1}(h_{i-1} + h_i)}(\psi_i - \psi_{i-1}) - n_i + p_i + C_i = 0 \quad (21)$$

ii) Electrons

$$\begin{aligned} & \frac{2\mu_{n,i+1/2}}{h_i(h_{i-1} + h_i)}B(\psi_{i+1} - \psi_i)n_{i+1} - \frac{2\mu_{n,i+1/2}}{h_i(h_{i-1} + h_i)}B(\psi_i - \psi_{i+1})n_i - \\ & \frac{2\mu_{n,i-1/2}}{h_{i-1}(h_{i-1} + h_i)}B(\psi_i - \psi_{i-1})n_i + \frac{2\mu_{n,i-1/2}}{h_{i-1}(h_{i-1} + h_i)}B(\psi_{i-1} - \psi_i)n_{i-1} - R(n_i, p_i) = 0 \end{aligned} \quad (22)$$

iii) Holes

$$\begin{aligned} & \frac{2\mu_{p,i+1/2}}{h_i(h_{i-1} + h_i)}B(\psi_i - \psi_{i+1})p_{i+1} - \frac{2\mu_{p,i+1/2}}{h_i(h_{i-1} + h_i)}B(\psi_{i+1} - \psi_i)p_i - \\ & \frac{2\mu_{p,i-1/2}}{h_{i-1}(h_{i-1} + h_i)}B(\psi_{i-1} - \psi_i)p_i + \frac{2\mu_{p,i-1/2}}{h_{i-1}(h_{i-1} + h_i)}B(\psi_i - \psi_{i-1})p_{i-1} + R(n_i, p_i) = 0 \end{aligned}$$

(23)

where, $B(x) = \frac{x}{\exp(x) - 1}$ is the Bernoulli's function. Yielding from this finite difference modelling is a large sparse nonlinear system of equations. The equations (21) – (23) are written in the residual form $\mathbf{F}_1(\psi, \mathbf{n}, \mathbf{p}) = 0$, $\mathbf{F}_2(\psi, \mathbf{n}, \mathbf{p}) = 0$, $\mathbf{F}_3(\psi, \mathbf{n}, \mathbf{p}) = 0$. The large sparse system of equations is then solved using Newton-like Gummel's iteration scheme. In the method,

i) a guess at the ψ is made,

ii) solve for hole quasi-Fermi potentials from the linearized continuity equations:

$$\text{div}[-\mu_n n \nabla \psi + \mu_n (\nabla \mathbf{d} \mathbf{n} - n \nabla \psi \mathbf{d} \mathbf{n})] - \frac{\partial R^k}{\partial n} \mathbf{d} \mathbf{n} - \frac{\partial R^k}{\partial p} \mathbf{d} \mathbf{p} + \text{div} \mathbf{J}_n^k - R^k = 0 \quad (24)$$

$$\text{div}[-\mu_p p \nabla \psi - (\nabla \mathbf{d} \mathbf{p} + n \nabla \psi \mathbf{d} \mathbf{p})] + \frac{\partial R^k}{\partial p} \mathbf{d} \mathbf{p} + \frac{\partial R^k}{\partial n} \mathbf{d} \mathbf{n} + \text{div} \mathbf{J}_p^k + R^k = 0 \quad (25)$$

where

$$\begin{aligned} \psi_{\text{new}} &= \psi + \mathbf{d} \psi \\ \mathbf{n}_{\text{new}} &= \mathbf{n} + \mathbf{d} \mathbf{n} \\ \mathbf{p}_{\text{new}} &= \mathbf{p} + \mathbf{d} \mathbf{p} \end{aligned} \quad (26)$$

iii) obtain a better approximation for ψ from Poisson's equation

$$\lambda^2 \Delta \mathbf{d} \psi + \lambda^2 \Delta \psi^k - (\mathbf{d} \mathbf{n} - \mathbf{d} \mathbf{p} - C) = 0 \quad (27)$$

4. Some Numerical Simulations

We have simulated a one dimensional pn-diode on the interval $[-1, 1]$. The scaled doping profile has an abrupt pn-junction at $x = 0$ which is defined as

$$C(x) = \begin{cases} 1 & -1 \leq x \leq 0 \\ -10^{-6} & 0 < x \leq 1 \end{cases}.$$

In equilibrium condition, no recombination and generation of the carriers are assumed. Computations are made for the forward bias of 30Volts. Dirichlet conditions hold at the boundaries ohmic contact while Neumann conditions hold at $x = -1$ and $x = 1$. Figure 1 shows how electric potentials vary with distances. Figure 2 shows the variation of electron concentrations with distances. Figure 3 gives the plot for variation of holes concentrations with distances. The results are obtained using the Newton-like Gummel's method after the nonlinear system has been linearized using the Newton-Raphson's linearization procedure. In the simulation we note to

- conserve the total number of particles inside the device simulated.
- respect local positivity of carrier density where negative density is unphysical.
- respect monotonicity of the solution (i.e. it should not introduce spurious space oscillations).

5. Conclusions

The equations (21) – (23) are written in the residual form $\mathbf{F}_1(\psi, \mathbf{n}, \mathbf{p}) = 0$, $\mathbf{F}_2(\psi, \mathbf{n}, \mathbf{p}) = 0$, $\mathbf{F}_3(\psi, \mathbf{n}, \mathbf{p}) = 0$. Newton-Raphson's linearization is made at $(\psi^k, \mathbf{n}^k, \mathbf{p}^k)$ which is

reasonably close to the solution, and is in the neighborhood where the solution is unique, Ithnin Abdul Jalil and Rio Hirowati Shariffudin (2005). The corrections $d\psi$, dn and dp are then calculated from the Jacobian system but in blocks after the matrix is split into blocks for the potential nodes, blocks for the electron concentration nodes and the blocks for the hole concentrations. For each block, finite difference modelling gives a tridiagonal system for a one dimensional problem. It is interesting to note that when two dimensional problem is to be solved the matrix may be decomposed such that we can have sets of potential nodes, sets of electron concentration nodes and sets of hole concentration nodes, Ithnin Abdul Jalil and Rio Hirowati Shariffudin (2004). Here, parallel computing fits in naturally and also communication issues that usually prevail in parallel computing are negligible or absent.

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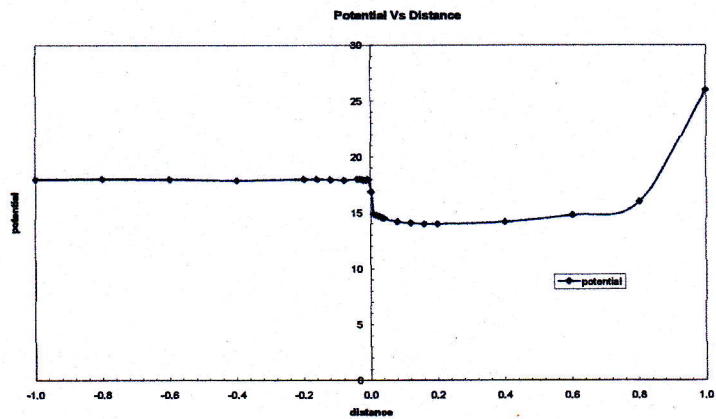


Figure 1: Variation of electric potential with distance

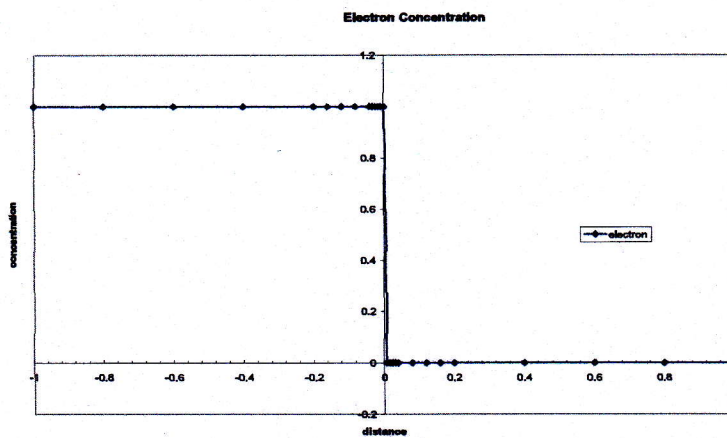


Figure 2: Variation of electron concentration with distance

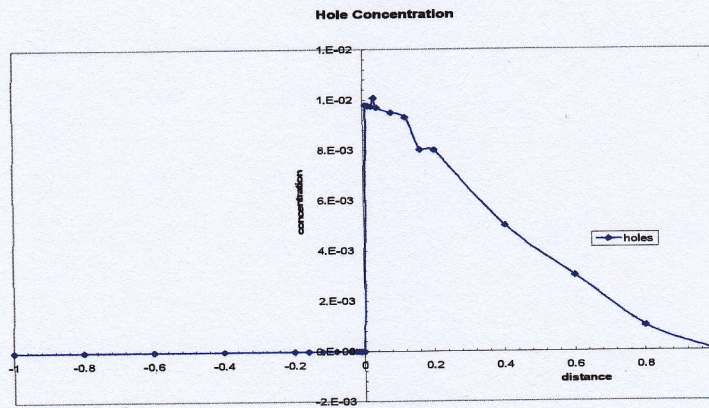


Figure 3: Variation hole concentration with distance

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